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FILE COVERS 1907 - 31 Jan 2003 VOL 138 ISS 6
FILE LAST UPDATED: 30 Jan 2003 (20030130/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

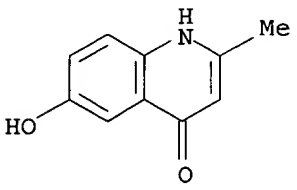
=> s l15
L16 180 L15

=> d abs ibib hitstr 160-180

L16 ANSWER 160 OF 180 CAPLUS COPYRIGHT 2003 ACS
GI For diagram(s), see printed CA Issue.
AB A soln. of 40 g I (R = Me) in 112 ml H2O and 200 ml H2SO4 was refl uxed 5 hr to yield 72.4% I (R = H) (II), m. 309-11.degree. (decompn.). II (1.0 g) and 0.51 g anhyd. AcOK in 5 ml Ac2O was refluxed 40 min t o yield 80% I (R = Ac), m. 257-8.degree. (EtOH). A soln. of 5 g Cu(OAc)2 in 50 ml MeOH contg. 5.4 g Me2NH was trea ted with 9.65 g II and the whole stirred with O bubbled through. In 3 hr 1650 ml O was consumed to yield 66.3% III (R = Me), (II ia) m. 177-8.degree. (decompn.) (EtOH). To a soln. of 2.5 g Cu(OAc)2 in 10 ml piperidine and 30 ml MeOH was added 4.83 g II and the whole stirred by bubbling in O; in 1.5 hr, 76 0 ml O was consumed to yield 61% III (NR2 = piperidino) (IV), m. 176-7.degree. (decompn.) (EtOH). To a refluxed soln. of 0.46 g IIIa in 2.5 ml EtOH was added 0.25 g o-phenylenediamine and the whole refluxed 10 min and kept 0.5 hr at room temp. to yield 66% V (R = NMe2), m. 162-3.degree. (Me2CO). Similarly, from IV, was obtained 98% V (R = piperidino), m. 209-10.degree. (PhMe). A suspension of 1.16 g IIIa in 10 ml EtOH was treated with 0.7 ml 80 % N2H4.H2O, and the whole refluxed 5 min to yield 71.4% VI (R = N me2), m. 223-5.degree. (50% EtOH). Similarly, 0.82 g IV and 0.44 g PhNHNH2.HCl gave 81% VI (R = piperidino), m. 240-2.degree.. To 13.9 g IIIa was added a mixt. of 50 ml EtOH and 125 ml N NaOH and the whole refluxed 15 min to yield 78% VII, m. >350.degree.. To a suspension of 0.45 g VII in 7 ml 60% AcOH at 60.degree. was added 0.25 g o-phenylenediamine and the whole refluxed 5 min to yield 63% V (R = OH), m. 253-5.degree. (HCONMe2). Ir, uv, and pKa data are given.

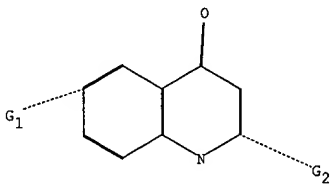
ACCESSION NUMBER: 1970:31563 CAPLUS
DOCUMENT NUMBER: 72:31563
TITLE: Heterocyclic quinones. III. Synthesis and properties of 2-methyl-4-hydroxy-8-dialkylamino-quinoline-5,6-quinones
AUTHOR(S): Tsizin, Yu. S.; Rubtsov, M. V.
CORPORATE SOURCE: Vses. Nauch.-Issled. Khim.-Farm. Inst., Moscow, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1969), (4), 682-6

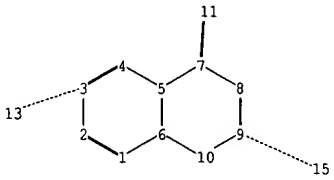
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT **15502-80-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 15502-80-4 CAPLUS
CN 4(1H)-Quinolone, 6-hydroxy-2-methyl- (8CI) (CA INDEX NAME)



L16 ANSWER 161 OF 180 CAPLUS COPYRIGHT 2003 ACS
AB Poly(oxoquinolines) are obtained by using a variation of the Von Niementowski reaction. A prior examn. of the simple anthranilic esters on the dioxolane of acetophenone shows that ethyl esters are much more suitable than methyl esters. A reaction was then set up between bisanthranilates (such as bis(2-aminoethyl) terephthalate and ethyl 4,4'-diamino-3,3'-biphenylyldicarboxylate and bisdioxolanes derived from diketones (such as diacetyl benzenes, bis(4-acetylphenyl) oxide or 4,4'-diacetylbiphenyl). Various solvents such as phenyl oxide and m-cresol, are used at their reflux temp. The inherent viscosities in HCO2H of the polymers thus obtained are of interest. Like their monomers, the polymers appear to exist in the solid state in a ketoquinoline form as shown by the ir spectrum. Thermogravimetric anal., from ambient temp. to 550.degree. in argon atm., recorded at a rate of 60.degree./hr., shows a decompn. of 5%.
ACCESSION NUMBER: 1969:422418 CAPLUS
DOCUMENT NUMBER: 71:22418
TITLE: Thermostable polymers. III. Poly(oxoquinolines)
AUTHOR(S): Sillion, Bernard; De Gaudemaris, Gabriel
CORPORATE SOURCE: Inst. Fr. Petrol., C.E.N., Grenoble, Fr.
SOURCE: Journal of Polymer Science, Polymer Symposia (1969), Volume Date 1965, No. 16(Pt. 8), 4653-67
CODEN: JPYCAQ; ISSN: 0360-8905
DOCUMENT TYPE: Journal
LANGUAGE: French
IT **24346-87-0**
RL: USES (Uses)
(model compds., from polymers of bisanthranilates with cyclic acetals of diketones)
RN 24346-87-0 CAPLUS
CN [6,6'-Biquinoline]-4,4'(1H,1'H)-dione, 2,2'-diphenyl- (8CI, 9CI) (CA INDEX NAME)

C:\Program Files\Stnexp\Queries\09840503.str





chain nodes :
11 13 15
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
3-13 7-11 9-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
3-13 5-7 6-10 7-8 7-11 8-9 9-10 9-15
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:CN,C,O,S,Hy

G2:C,Cy

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
13:CLASS 15:CLASS

Connecting via Winsock to STN

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	Apr 08	"Ask CAS" for self-help around the clock
NEWS 3	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4	Apr 09	ZDB will be removed from STN
NEWS 5	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 7	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS 8	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS 9	Jun 03	New e-mail delivery for search results now available
NEWS 10	Jun 10	MEDLINE Reload
NEWS 11	Jun 10	PCTFULL has been reloaded
NEWS 12	Jul 02	FOREGE no longer contains STANDARDS file segment
NEWS 13	Jul 22	USAN to be reloaded July 28, 2002; saved answer sets no longer valid
NEWS 14	Jul 29	Enhanced polymer searching in REGISTRY
NEWS 15	Jul 30	NETFIRST to be removed from STN
NEWS 16	Aug 08	CANCERLIT reload
NEWS 17	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18	Aug 08	NTIS has been reloaded and enhanced
NEWS 19	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 20	Aug 19	IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21	Aug 19	The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 23	Sep 03	JAPIO has been reloaded and enhanced
NEWS 24	Sep 16	Experimental properties added to the REGISTRY file
NEWS 25	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 26	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 27	Oct 21	EVENTLINE has been reloaded
NEWS 28	Oct 24	BEILSTEIN adds new search fields
NEWS 29	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 30	Oct 25	MEDLINE SDI run of October 8, 2002
NEWS 31	Nov 18	DKILIT has been renamed APOLLIT
NEWS 32	Nov 25	More calculated properties added to REGISTRY
NEWS 33	Dec 02	TIBKAT will be removed from STN
NEWS 34	Dec 04	CSA files on STN
NEWS 35	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 36	Dec 17	TOXCENTER enhanced with additional content
NEWS 37	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 38	Dec 30	ISMEC no longer available
NEWS 39	Jan 13	Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 40	Jan 21	NUTRACEUT offering one free connect hour in February 2003
NEWS 41	Jan 21	PHARMAML offering one free connect hour in February 2003

NEWS 42 Jan 29 Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC

NEWS EXPRESS January 6 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
NEWS HOURS STN Operating Hours Plus Help Desk Availability
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NEWS WWW CAS World Wide Web Site (general information)

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* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:39:23 ON 31 JAN 2003

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 10:39:30 ON 31 JAN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 JAN 2003 HIGHEST RN 483275-57-6
DICTIONARY FILE UPDATES: 29 JAN 2003 HIGHEST RN 483275-57-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

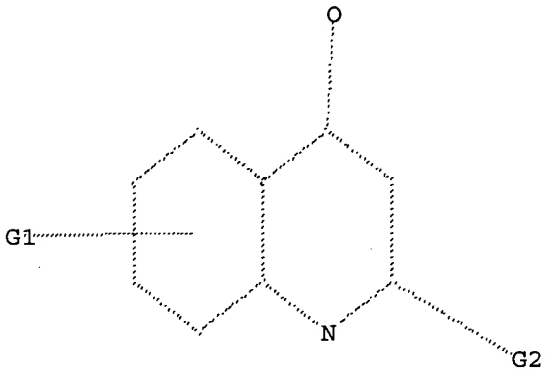
=> d l1
NO L# DEFINED

There are no L# queries, structures, or screen sets
defined in the current session.

=>
Uploading 09840503.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 CN,C,O,S,Hy
G2 C,Cy

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 10:40:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 21120 TO ITERATE

4.7% PROCESSED 1000 ITERATIONS 16 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 413721 TO 431079
PROJECTED ANSWERS: 5656 TO 7860

L2 16 SEA SSS SAM L1

=>
=> s nc5-c6/es
L3 488273 NC5-C6/ES

=> s l1 sub=l3
ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):s
'S' IS NOT A VALID SUBSET SEARCH SCOPE
For an explanation, enter "HELP SEARCH SCOPES".

=> s l1 sub=l3
ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):sample

SAMPLE SUBSET SEARCH INITIATED 10:42:41 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED - 5187 TO ITERATE

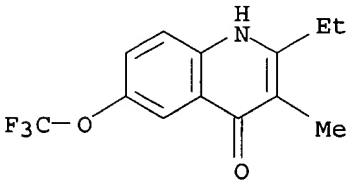
19.3% PROCESSED 1000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): 99424 TO 108056
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 6693 TO 9075

L4 50 SEA SUB=L3 SSS SAM L1

=> d scan

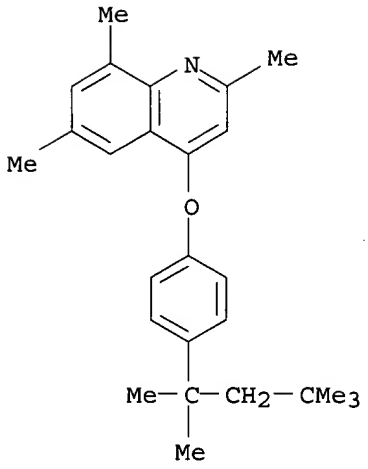
L4 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 4(1H)-Quinolinone, 2-ethyl-3-methyl-6-(trifluoromethoxy)- (9CI)
MF C13 H12 F3 N O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

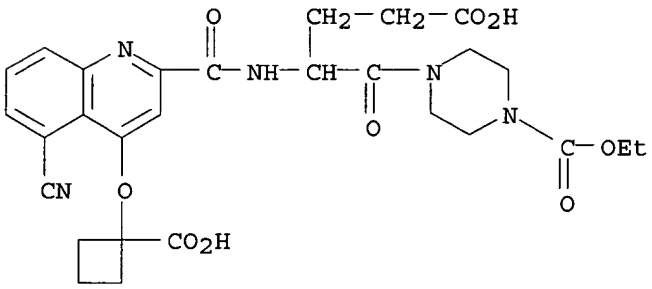
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L4 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Quinoline, 2,6,8-trimethyl-4-[4-(1,1,3,3-tetramethylbutyl)phenoxy]- (9CI)
MF C26 H33 N O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

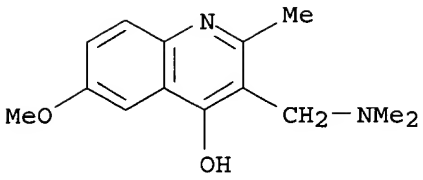
L4 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 1-Piperazinepentanoic acid, .gamma.-[[[4-[(1-carboxycyclobutyl)oxy]-5-cyano-2-quinolinyl]carbonyl]amino]-4-(ethoxycarbonyl)-.delta.-oxo- (9CI)
MF C28 H31 N5 O9



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

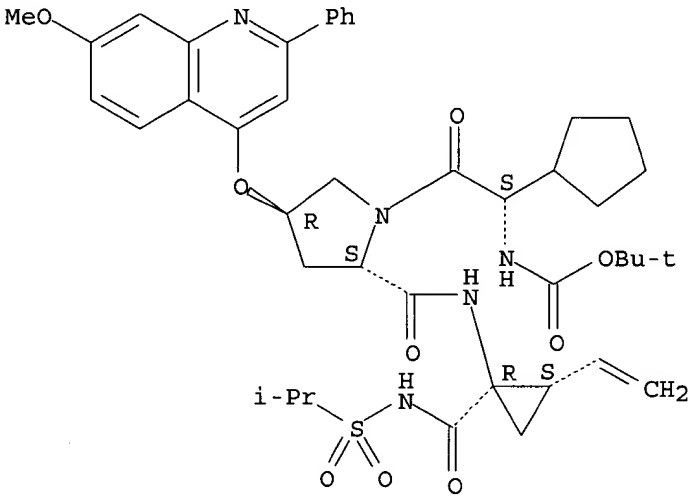
L4 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 4-Quinolinol, 3-[(dimethylamino)methyl]-6-methoxy-2-methyl- (9CI)
MF C14 H18 N2 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Cyclopropanecarboxamide, (2S)-2-cyclopentyl-N-[(1,1-dimethylethoxy)carbonyl]glycyl-(4R)-4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]-L-prolyl-1-amino-2-ethenyl-N-[(1-methylethyl)sulfonyl]-, (1R,2S)- (9CI)
MF C42 H53 N5 O9 S

Absolute stereochemistry.



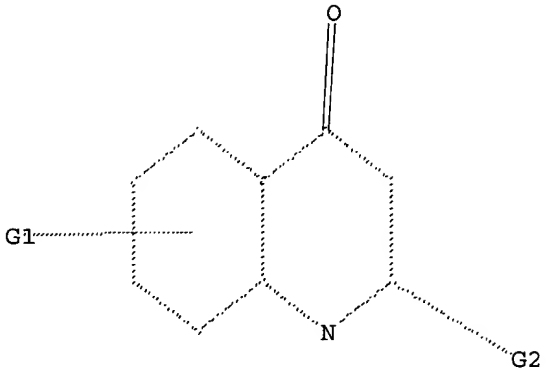
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=>
Uploading 09840503.str

L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR



G1 CN,C,O,S,Hy

G2 C,Cy

Structure attributes must be viewed using STN Express query preparation.

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=> s l5
SAMPLE SEARCH INITIATED 10:46:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  21120 TO ITERATE

  4.7% PROCESSED    1000 ITERATIONS                                  6 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       413721 TO   431079
PROJECTED ANSWERS:            1859 TO     3209

L6            6 SEA SSS SAM L5

=>
Uploading 09840503.str

L7      STRUCTURE UPLOADED

=> d l7
L7 HAS NO ANSWERS
L7              STR
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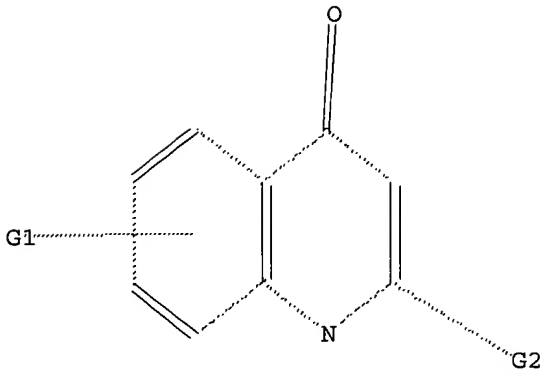
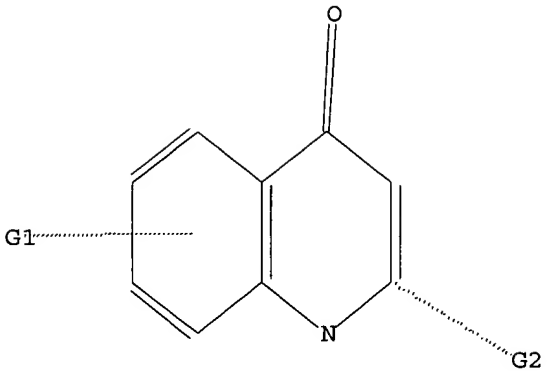


G1 CN,C,O,S,Hy

G2 C,Cy

Structure attributes must be viewed using STN Express query preparation.

```
=> s l7
SAMPLE SEARCH INITIATED 10:47:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  21120 TO ITERATE

  4.7% PROCESSED    1000 ITERATIONS                                5 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       413721 TO   431079
PROJECTED ANSWERS:            1496 TO     2728

L8            5 SEA SSS SAM L7

=>
Uploading 09840503.str

L9      STRUCTURE UPLOADED

=> d l9
L9 HAS NO ANSWERS
L9              STR
```

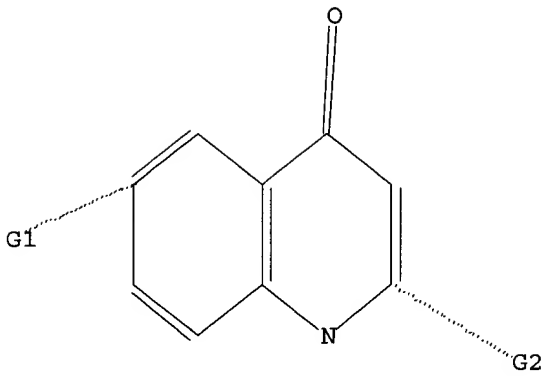


G1 CN,C,O,S,Hy

G2 C,Cy

Structure attributes must be viewed using STN Express query preparation.

```
=> s l9
SAMPLE SEARCH INITIATED 10:48:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  21120 TO ITERATE

  4.7% PROCESSED    1000 ITERATIONS                                5 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       413721 TO   431079
PROJECTED ANSWERS:            1496 TO     2728

L10           5 SEA SSS SAM L9

=>
Uploading 09840503.str

L11     STRUCTURE UPLOADED

=> d l11
L11 HAS NO ANSWERS
L11             STR
```

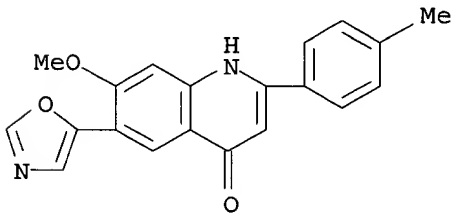


G1 CN,C,O,S,Hy

G2 C,Cy

Structure attributes must be viewed using STN Express query preparation.

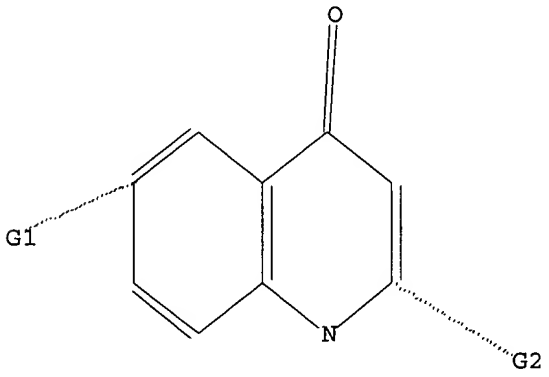
```
=> s l11
SAMPLE SEARCH INITIATED 10:49:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  16045 TO ITERATE

  6.2% PROCESSED    1000 ITERATIONS                                5 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       313327 TO   328473
PROJECTED ANSWERS:            1067 TO     2141

L12           5 SEA SSS SAM L11

=> d scan

L12  5 ANSWERS   REGISTRY  COPYRIGHT 2003 ACS
IN   4(1H)-Quinolinone, 7-methoxy-2-(4-methylphenyl)-6-(5-oxazolyl)- (9CI)
MF   C20 H16 N2 O3
```



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> s l11 ful
FULL SEARCH INITIATED 10:50:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 320838 TO ITERATE

100.0% PROCESSED  320838 ITERATIONS                      1125 ANSWERS
SEARCH TIME: 00.00.06

L13         1125 SEA SSS FUL L11

=>
Uploading 09840503.str

L14      STRUCTURE UPLOADED

=> d l14
L14 HAS NO ANSWERS
L14              STR
```

R groups can form further ring
Searches were saved for future use




```
G1 CN,C,O,S,Hy
G2 C,Cy


Structure attributes must be viewed using STN Express query preparation.


=> s l14 ful sub=l13
FULL SUBSET SEARCH INITIATED 10:52:05 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -   1085 TO ITERATE

100.0% PROCESSED    1085 ITERATIONS                      1069 ANSWERS
SEARCH TIME: 00.00.01

L15         1069 SEA SUB=L13 SSS FUL L14

=> fil caplus
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                              ENTRY    SESSION
FULL ESTIMATED COST                           195.27     195.48

FILE 'CAPLUS' ENTERED AT 10:52:15 ON 31 JAN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
```

R groups cannot form further ring
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FILE LAST UPDATED: 30 Jan 2003 (20030130/ED)

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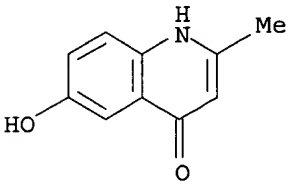
=> s l15
L16 180 L15

=> d abs ibib hitstr 160-180

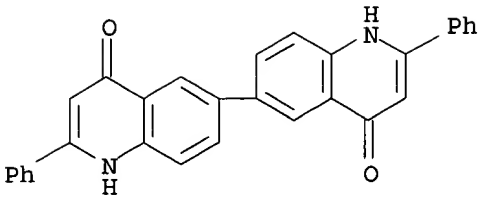
L16 ANSWER 160 OF 180 CAPLUS COPYRIGHT 2003 ACS
GI For diagram(s), see printed CA Issue.
AB A soln. of 40 g I (R = Me) in 112 ml H2O and 200 ml H2SO4 was refl uxed 5 hr to yield 72.4% I (R = H) (II), m. 309-11.degree. (decompn.). II (1.0 g) and 0.51 g anhyd. AcOK in 5 ml Ac2O was refluxed 40 min t o yield 80% I (R = Ac), m. 257-8.degree. (EtOH). A soln. of 5 g Cu(OAc)2 in 50 ml MeOH contg. 5.4 g Me2NH was trea ted with 9.65 g II and the whole stirred with O bubbled through. In 3 hr 1650 ml O was consumed to yield 66.3% III (R = Me), (II ia) m. 177-8.degree. (decompn.) (EtOH). To a soln. of 2.5 g Cu(OAc)2 in 10 ml piperidine and 30 ml MeOH was added 4.83 g II and the whole stirred by bubbling in O; in 1.5 hr, 76 0 ml O was consumed to yield 61% III (NR2 = piperidino) (IV), m. 176-7.degree. (decompn.) (EtOH). To a refluxed soln. of 0.46 g IIIa in 2.5 ml EtOH was added 0.25 g o-phenylenediamine and the whole refluxed 10 min and kept 0.5 hr at room temp. to yield 66% V (R = NMe2), m. 162-3.degree. (Me2CO). Similarly, from IV, was obtained 98% V (R = piperidino), m. 209-10.degree. (PhMe). A suspension of 1.16 g IIIa in 10 ml EtOH was treated with 0.7 ml 80 % N2H4.H2O, and the whole refluxed 5 min to yield 71.4% VI (R = N me2), m. 223-5.degree. (50% EtOH). Similarly, 0.82 g IV and 0.44 g PhNHNH2.HCl gave 81% VI (R = piperidino), m. 240-2.degree.. To 13.9 g IIIa was added a mixt. of 50 ml EtOH and 125 ml N NaOH and the whole refluxed 15 min to yield 78% VII, m. >350.degree.. To a suspension of 0.45 g VII in 7 ml 60% AcOH at 60.degree. was added 0.25 g o-phenylenediamine and the whole refluxed 5 min to yield 63% V (R = OH), m. 253-5.degree. (HCONMe2). Ir, uv, and pKa data are given.

ACCESSION NUMBER: 1970:31563 CAPLUS
DOCUMENT NUMBER: 72:31563
TITLE: Heterocyclic quinones. III. Synthesis and properties of 2-methyl-4-hydroxy-8-dialkylamino-quinoline-5,6-quinones
AUTHOR(S): Tsizin, Yu. S.; Rubtsov, M. V.
CORPORATE SOURCE: Vses. Nauch.-Issled. Khim.-Farm. Inst., Moscow, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1969), (4), 682-6

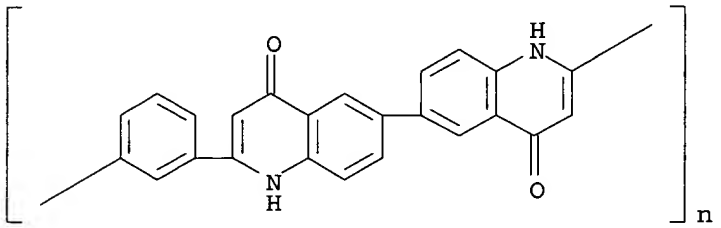
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT **15502-80-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 15502-80-4 CAPLUS
CN 4(1H)-Quinolone, 6-hydroxy-2-methyl- (8CI) (CA INDEX NAME)



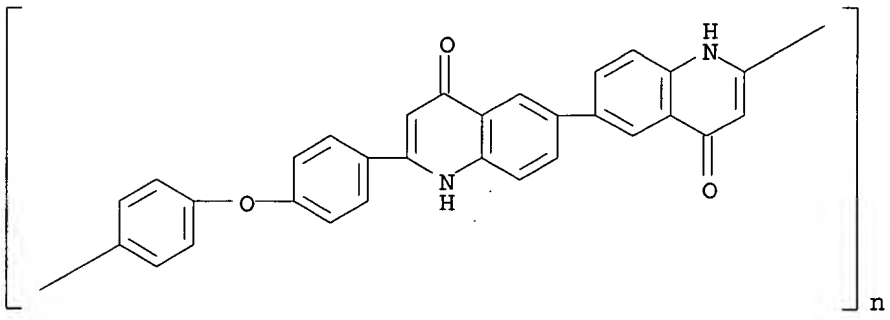
L16 ANSWER 161 OF 180 CAPLUS COPYRIGHT 2003 ACS
AB Poly(oxoquinolines) are obtained by using a variation of the Von Niementowski reaction. A prior examn. of the simple anthranilic esters on the dioxolane of acetophenone shows that ethyl esters are much more suitable than methyl esters. A reaction was then set up between bisanthranilates (such as bis(2-aminoethyl) terephthalate and ethyl 4,4'-diamino-3,3'-biphenylyldicarboxylate and bisdioxolanes derived from diketones (such as diacetyl benzenes, bis(4-acetylphenyl) oxide or 4,4'-diacetylbiphenyl). Various solvents such as phenyl oxide and m-cresol, are used at their reflux temp. The inherent viscosities in HCO2H of the polymers thus obtained are of interest. Like their monomers, the polymers appear to exist in the solid state in a ketoquinoline form as shown by the ir spectrum. Thermogravimetric anal., from ambient temp. to 550.degree. in argon atm., recorded at a rate of 60.degree./hr., shows a decompn. of 5%.
ACCESSION NUMBER: 1969:422418 CAPLUS
DOCUMENT NUMBER: 71:22418
TITLE: Thermostable polymers. III. Poly(oxoquinolines)
AUTHOR(S): Sillion, Bernard; De Gaudemaris, Gabriel
CORPORATE SOURCE: Inst. Fr. Petrol., C.E.N., Grenoble, Fr.
SOURCE: Journal of Polymer Science, Polymer Symposia (1969), Volume Date 1965, No. 16(Pt. 8), 4653-67
CODEN: JPYCAQ; ISSN: 0360-8905
DOCUMENT TYPE: Journal
LANGUAGE: French
IT **24346-87-0**
RL: USES (Uses)
(model compds., from polymers of bisanthranilates with cyclic acetals of diketones)
RN 24346-87-0 CAPLUS
CN [6,6'-Biquinoline]-4,4'(1H,1'H)-dione, 2,2'-diphenyl- (8CI, 9CI) (CA INDEX NAME)



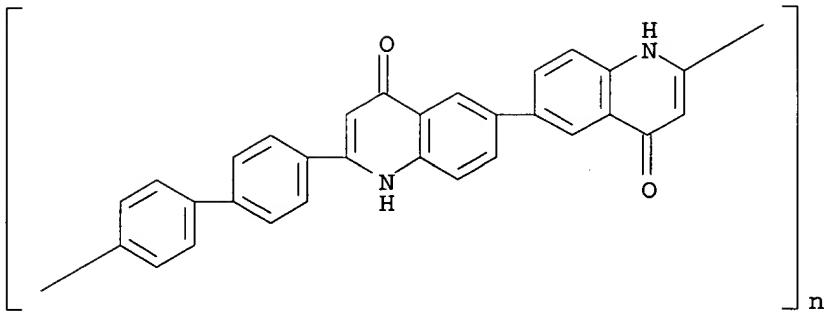
IT **26917-37-3P 26917-38-4P 26917-39-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 26917-37-3 CAPLUS
CN Poly[(1,1',4,4'-tetrahydro-4,4'-dioxo[6,6'-biquinoline]-2,2'-diyl)-m-phenylene] (8CI) (CA INDEX NAME)



RN 26917-38-4 CAPLUS
CN Poly[(1,1',4,4'-tetrahydro-4,4'-dioxo[6,6'-biquinoline]-2,2'-diyl)-p-phenyleneoxy-p-phenylene] (8CI) (CA INDEX NAME)



RN 26917-39-5 CAPLUS
CN Poly[(1,1',4,4'-tetrahydro-4,4'-dioxo[6,6'-biquinoline]-2,2'-diyl)-4,4'-biphenylylene] (8CI) (CA INDEX NAME)

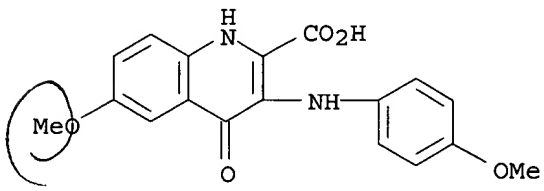


L16 ANSWER 162 OF 180 CAPLUS COPYRIGHT 2003 ACS
GI For diagram(s), see printed CA Issue.
AB Two new syntheses of epindolidione (I) are described. The first synthesis affords I and some sym. substituted derivs. in good yield and relatively high purity. Di-Me dihydroxyfumarate reacts with aniline to give di-Me dianilinomaleate (II). Evidence for the cis structure of II is given. II is cyclized to 2-methoxycarbonyl-3-anilino-4-quinolone which in turn is cyclized to I. The second method involves the cyclization of 3-(2-carboxyphenylamino)-4-quinolone which is obtained by condensation of 3-amino-4-quinolone with o-bromobenzoic acid. Phys. and spectral properties of I are discussed and evidence for intermol. bonding is presented. 28 references.

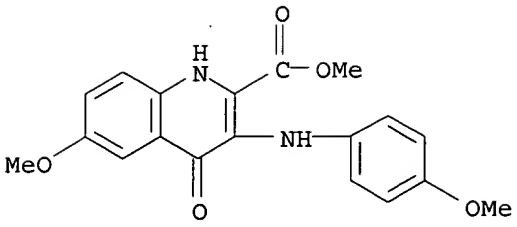
ACCESSION NUMBER: 1969:11596 CAPLUS
DOCUMENT NUMBER: 70:11596
TITLE: Synthesis of epindolidione
AUTHOR(S): Jaffe, Edward E.; Matrick, Howard
CORPORATE SOURCE: Pigments Dep., E. I. du Pont de Nemours and Co., Newark, NJ, USA
SOURCE: Journal of Organic Chemistry (1968), 33(11), 4004-10
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **16377-61-0P 16479-61-1P 17540-32-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

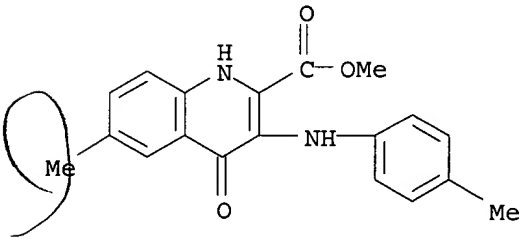
RN 16377-61-0 CAPLUS
CN Quinaldic acid, 3-p-anisidino-1,4-dihydro-6-methoxy-4-oxo- (8CI) (CA INDEX NAME)



RN 16479-61-1 CAPLUS
CN Quinaldic acid, 3-p-anisidino-1,4-dihydro-6-methoxy-4-oxo-, methyl ester (8CI) (CA INDEX NAME)

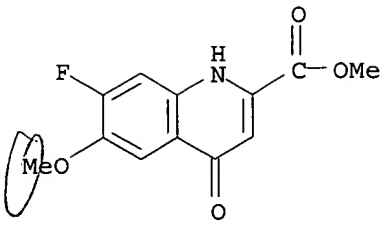


RN 17540-32-8 CAPLUS
CN Quinaldic acid, 1,4-dihydro-6-methyl-4-oxo-3-p-toluidino-, methyl ester (8CI) (CA INDEX NAME)

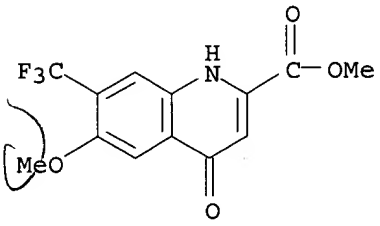


L16 ANSWER 163 OF 180 CAPLUS COPYRIGHT 2003 ACS
GI For diagram(s), see printed CA Issue.
AB Substituted anilines and MeO2CC.tplbond.CCO2Me are condensed to prep. 9 di-Me anilino-fumarates (I) which are subjected to ring closure to prep. 4(1H)-quinolone-2-carboxylates (II). None of the fumarates and quinolones showed any significant antimalarial activity against Plasmodium berghei in mice.

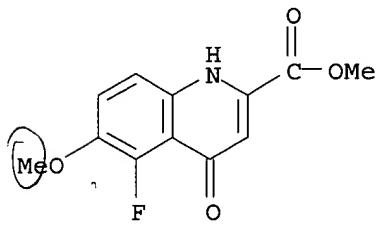
ACCESSION NUMBER: 1969:11538 CAPLUS
DOCUMENT NUMBER: 70:11538
TITLE: Cyclization of aniline-acetylenedicarboxylate adducts. A modified Conrad-Limpach method for the synthesis of potential antimalarials
AUTHOR(S): Heindel, Ned D.; Bechara, Ibrahim S.; Kennewell, Peter D.; Molnar, James; Ohnmacht, Cyrus J.; Lemke, Sally M.; Lemke, Thomas F.
CORPORATE SOURCE: Lehigh Univ., Bethlehem, PA, USA
SOURCE: Journal of Medicinal Chemistry (1968), 11(6), 1218-21
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **19271-20-6P 19271-21-7P 19298-74-9P 20843-50-9P 20843-51-0P 20843-54-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 19271-20-6 CAPLUS
CN 2-Quinolinecarboxylic acid, 7-fluoro-1,4-dihydro-6-methoxy-4-oxo-, methyl ester (9CI) (CA INDEX NAME)



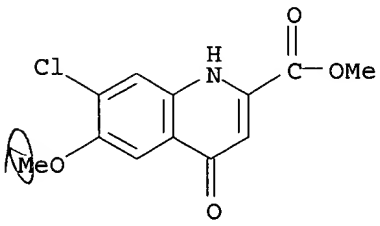
RN 19271-21-7 CAPLUS
CN 2-Quinolinecarboxylic acid, 1,4-dihydro-6-methoxy-4-oxo-7-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



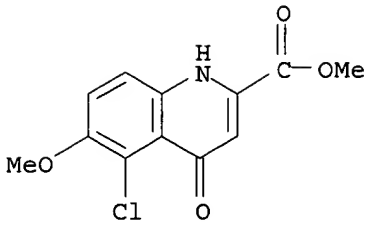
RN 19298-74-9 CAPLUS
CN 2-Quinolinecarboxylic acid, 5-fluoro-1,4-dihydro-6-methoxy-4-oxo-, methyl ester (9CI) (CA INDEX NAME)



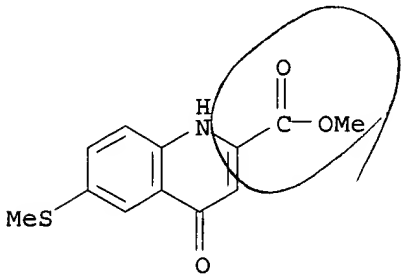
RN 20843-50-9 CAPLUS
CN Quinaldic acid, 7-chloro-1,4-dihydro-6-methoxy-4-oxo-, methyl ester (8CI) (CA INDEX NAME)



RN 20843-51-0 CAPLUS
CN Quinaldic acid, 5-chloro-1,4-dihydro-6-methoxy-4-oxo-, methyl ester (8CI) (CA INDEX NAME)

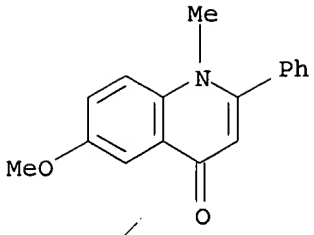


RN 20843-54-3 CAPLUS
CN 2-Quinolinecarboxylic acid, 1,4-dihydro-6-(methylthio)-4-oxo-, methyl ester (9CI) (CA INDEX NAME)



L16 ANSWER 164 OF 180 CAPLUS COPYRIGHT 2003 ACS
GI For diagram(s), see printed CA Issue.
AB Seed exts. of C. edulis yielded 5-methoxy-8-geranyloxypsoralen, phellopterin, zapotin, 2',5,6-trimethoxyflavone, 3',5,6-trimethoxyflavone (I), 3',5,5',6-tetramethoxyflavone (II), casimiroin, eduline, eduline, 1-methyl-2-phenyl-4-quinolone, zapoterin (III), 7.alpha.-obacunol, and deacetylnomilin. III is a C26 limonoid and was converted into a monoacetate and oxidized to a ketone, zapoterone, with chromic acid. These chem. transformations and spectroscopic considerations indicate III is 12.alpha.-hydroxyobacunone. The synthesis of I and II is also reported.

ACCESSION NUMBER: 1968:467555 CAPLUS
DOCUMENT NUMBER: 69:67555
TITLE: Citrus bitter principles. IX. Extractives of Casimiroa edulis. Structure of zapoterin
AUTHOR(S): Dreyer, David L.
CORPORATE SOURCE: Fruit and Veg. Chem. Lab., Pasadena, CA, USA
SOURCE: Journal of Organic Chemistry (1968), 33(9), 3577-82
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **6878-08-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 6878-08-6 CAPLUS
CN 4(1H)-Quinolinone, 6-methoxy-1-methyl-2-phenyl- (9CI) (CA INDEX NAME)



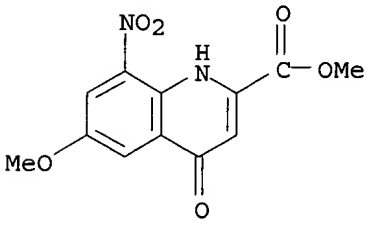
L16 ANSWER 165 OF 180 CAPLUS COPYRIGHT 2003 ACS

AB 8-Nitro-2-carbomethoxy-4(1H)-quinolones (I) were obtained by Michael condensation of o-nitroanilines with MeO2CC.tplbond.CCO2Me, followed by cyclization with polyphosphoric acid. I were easily sapond. and decarboxylated. The mechanism of the formation of I is discussed.

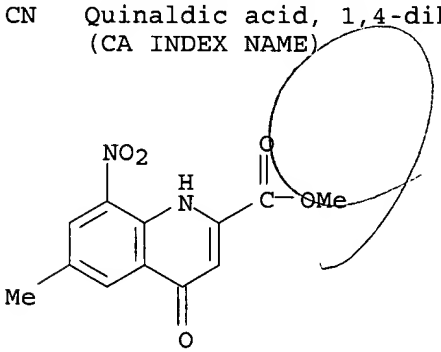
ACCESSION NUMBER: 1968:29560 CAPLUS
DOCUMENT NUMBER: 68:29560
TITLE: Cyclization of aniline-acetylenedicarboxylate adducts. Improved synthesis of 8-nitro-2-carbomethoxy-4(1H)-quinolones
AUTHOR(S): Heindel, Ned D.; Bechara, Ibrahim S.; Lemke, Thomas F.; Fish, Velmer B.
CORPORATE SOURCE: Lehigh Univ., Bethlehem, PA, USA
SOURCE: Journal of Organic Chemistry (1967), 32(12), 4155-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

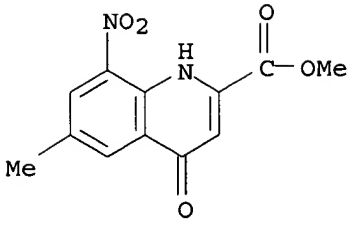
IT **16134-02-4P 16134-04-6P 16134-05-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 16134-02-4 CAPLUS
CN Quinaldic acid, 1,4-dihydro-6-methoxy-8-nitro-4-oxo-, methyl ester (8CI) (CA INDEX NAME)

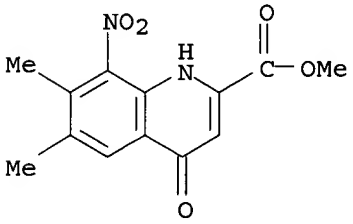


RN 16134-04-6 CAPLUS
CN Quinaldic acid, 1,4-dihydro-6-methyl-8-nitro-4-oxo-, methyl ester (8CI) (CA INDEX NAME)



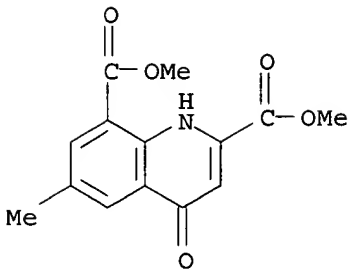


RN 16134-05-7 CAPLUS
CN Quinaldic acid, 1,4-dihydro-6,7-dimethyl-8-nitro-4-oxo-, methyl ester (8CI) (CA INDEX NAME)



L16 ANSWER 166 OF 180 CAPLUS COPYRIGHT 2003 ACS
GI For diagram(s), see printed CA Issue.
AB Isatoic anhydrides and anthranilic esters react with acetylenedicarboxylates to give Michael adducts (I) which cyclize to 2,8-dicarboalkoxy-4-(1H)-quinolinones (II) upon heating. The synthesis is limited by steric and electronic features in the initial anhydrides and esters which inhibit formation of the intermediate enamines. 24 references.

ACCESSION NUMBER: 1968:2792 CAPLUS
DOCUMENT NUMBER: 68:2792
TITLE: Cyclizations of anthranilate-acetylenedicarboxylate adducts. A facile route to 2,8-dicarboalkoxy-4(1H)quinolinones
AUTHOR(S): Taylor, Edward Curtis; Heindel, Ned D.
CORPORATE SOURCE: Princeton Univ., Princeton, NJ, USA
SOURCE: Journal of Organic Chemistry (1967), 32(11), 3339-43
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **14320-46-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 14320-46-8 CAPLUS
CN 2,8-Quinolinedicarboxylic acid, 1,4-dihydro-6-methyl-4-oxo-, dimethyl ester (8CI) (CA INDEX NAME)

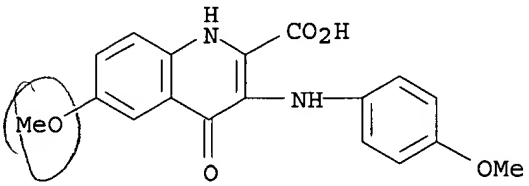


L16 ANSWER 167 OF 180 CAPLUS COPYRIGHT 2003 ACS
GI For diagram(s), see printed CA Issue.
AB Compds. of the general formula I are prepd. by condensing trans-(MeO2CC(OH):)2 (II) with the appropriate aniline in an inert org. solvent in the presence of an acid catalyst to form III, cyclizing III to IV by heating at 225-300.degree. in Downtherm A (23.5% Ph2-76.5% Ph2O) (V) and further cyclizing IV at 90-175.degree. in the presence of polyphosphoric acid (82-4% P2O5) (PPA) to give I. For example, a mixt. of II 66, MeOH 320, PhNH2 77, and PhNH2.HCl 7.5 parts is heated under reflux for .apprx.5.5 hrs. and cooled to room temp. to give 102 parts (83.4%) III (X = Y = H) (VI), m. 195-6.degree. (BuOH). Similarly, other III are prepd. (X, Y, % yield, and m.p. given): Cl, H, 85, 194.5-5.5.degree.; Cl, Cl, 89, -; H, Cl, 99, 138-40.5.degree.; Br, H, 79, 201-3.degree.; MeO, H, 45, 133-7.degree.. A mixt. of 50 parts VI and 500 parts V is stirred and heated rapidly to 250.degree., held for 5 min., and cooled to 10.degree. to give 35 parts (77.6% yield) yellow cryst. IV (X = Y = H) (VII), m. 193-4.degree. (MeOH). Similarly, other IV are prepd. (X, Y, % yield, and m.p. given): Cl, H, 89, 244-7.degree.; Cl, Cl 90, -; H, Cl, 97, -; Br, H, 92, 259-62.degree.; MeO, H, 70, 222-6.degree. [free acid m. 205.degree. (decomp.)]. A mixt. of 79 parts VII and 790 parts PPA is heated to 150.degree. during 1 hr., held at 145-50.degree. for 2 hrs., cooled to 40-50.degree. and treated slowly with H2O as the temp. is held at 50.degree.. After the vigorous reaction ceases, excess H2O is added to give 70 parts (100% yield) I (X = Y = H), a high strength yellow pigment of excellent durability. Similarly, other I are prepd. (X, Y, % yield, and shade given): Cl, H, 97, yellow; F, H, -, yellow; Cl, Cl, 100, greenish yellow; H, Cl, -, greenish yellow; Br, H, 84, greenish yellow (m. >400.degree.); MeO, H, 80, reddish yellow. A soln. of 210 parts EtO2CCOCH(Na)CO2Et in C6H6 is treated with 500 parts H2O at 7-10.degree. and with 1000 parts C6H6, stirred well, slowly acidified with dil. HCl until the pH of the aq. phase is >7, the C6H6 phase sepd., extd. with H2O to remove acid, treated with 113 parts 4-FC6H4NH2 (VIII), refluxed for 4 hrs. with H2O-sepn., cooled, excess VIII extd. with 2 .times. 150 parts 6N HCl, washed acid-free and the C6H6 distd. to give 4-FC6H4NHC(CO2Et):CHCO2Et (IX). Cyclization of IX by heating in V at 250-3.degree. gives 55% X (X = F, Y = H, R = OEt), m. 239-40.degree. (EtOH), which is chlorinated with SO2Cl2 in Ac2O-AcOH to give 86% X (X = F, Y = Cl, R = OEt) (XI). Treatment of XI with PhNH2 at 145-50.degree. in the presence of KOAc and Cu(OAc)2 gives 58% X (X = F, Y = R = NHPh) which is cyclized with PPA to give 72% I (one X = F, other X and Y = H), bright yellow powder, decomp. 400-50.degree.. Similarly are prepd. X (X = Y = H, R = OEt), m. 204-8.degree., X (X = H, Y = Cl, R = OEt), m. 213-16.degree., X (X = H, Y = R = NHC6H4Cl-4), X (X = H, Y = NHC6H4Cl-4, R = OH), and I (one X = Cl, other X and Y = H), bright yellow.
ACCESSION NUMBER: 1967:509632 CAPLUS
DOCUMENT NUMBER: 67:109632

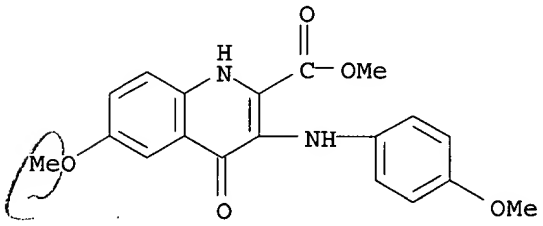
TITLE: Quinolonoquinolone pigments
INVENTOR(S): Aldridge, Gerald R.; Jaffe, Edward E.; Matrick, Howard
PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co.
SOURCE: U.S., 9 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3334102		19670801	US	19640227

IT **16377-61-0P 16479-61-1P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(prepn. of)
RN 16377-61-0 CAPLUS
CN Quinaldic acid, 3-p-anisidino-1,4-dihydro-6-methoxy-4-oxo- (8CI) (CA INDEX NAME)



RN 16479-61-1 CAPLUS
CN Quinaldic acid, 3-p-anisidino-1,4-dihydro-6-methoxy-4-oxo-, methyl ester (8CI) (CA INDEX NAME)



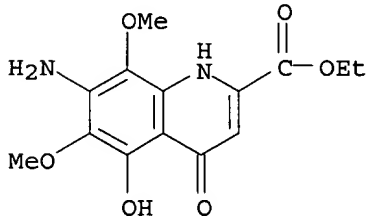
L16 ANSWER 168 OF 180 CAPLUS COPYRIGHT 2003 ACS
GI For diagram(s), see printed CA Issue.
AB cf. preceding abstr. Compds. of the general formula I are treated at .apprx.200.degree. with S to give mixts. contg. compds. of the general formula II (X = S) and III. Small dipole moment values are obtained for the III; the presence of O-S bonds (IV) is suggested. Thus, o-MeOC6H4CHO is condensed with AcH to give 57% o-MeOC6H4CH:CHCHO, b13 163-5.degree., m. 45-6.degree.. Similarly prepd. are the following ArCH:CHCHO (Ar, b.p./mm., and m.p. given): p-MeOC6H4, 170-5.degree./13, 57-9.degree.; 2,3-(MeO)2C6H3, 160.degree./5, 77.5.degree.; 3,4-(MeO)2C6H3, 170-90.degree./13, 81.degree.; 3,4-methylenedioxyphenyl, 190-210.degree./12, 85.degree.; p-tolyl, 154-9.degree./25, 41.5.degree.; 2-furyl, 105-10.degree./13, 51.degree.; 2-thienyl, 95.degree./1, -. A

mixt. of 0.1 mole 1-tetralone, 0.12 mole PhCH:CHCHO, and 50 ml. 4% KOH (alc.) is kept 1 hr. to give I (Ar = Ph) (V), m. 134.degree.. Similarly prepd. are the following I (Ar and m.p. given): o-MeOC6H4, 130.degree.; p-MeOC6H4, 146.degree.; 2,3-(MeO)2C6H3, 123.5.degree.; 3,4-(MeO)2C6H3, 129.5.degree.; 3,4-(methylenedioxy)phenyl, 172.degree.; p-tolyl, 152.degree.; 2-furyl, 98.degree.; 2-thenyl, 128.degree.. A mixt. of 20 g. V and 30 g. S is heated 1 hr. at 200-10.degree. to give a mixt. of 2-phenylbenzo[h]chromene-4-thione (II, Ar = Ph, X = S) (VI), 173.5.degree., and 2-(5-phenyl-1,2-dithiole-3-ylio)naphtholate (III, Ar = Ph) (VIa), m. 180.degree.. Similarly prepd. are the following II (X = S)-III mixts. (Ar, m.p. II, and m.p. III given): o-MeOC6H4, 177.5.degree., 139.degree.; p-MeOC6H4, 224.degree., 218-19.degree.; 2,3-(MeO)2C6H3, 149.5.degree., -; 3,4-(MeO)2C6H3, 203.degree., 179.degree.; 3,4-(methylenedioxy)phenyl, 253.degree., 208.degree.; p-tolyl, 190.degree., 186.5.degree., 2-furyl, 173.degree., 197-8.degree.; 2-thienyl, 189.degree., 192.5.degree.. VI is treated with KMnO4 to give 2-phenylbenzo[h]chromen-4-one (II, X = O, Ar = Ph), m. 154.degree.. Similarly prepd. are the following II (X = O) (Ar and m.p. given): o-MeOC6H4, 164.degree.; p-MeOC6H4, 184.degree.; 2,3-(MeO)2C6H3, 147.degree. and 152.5.degree.; 3,4-(MeO)2C6H3, 190.degree.; 3,4-(methylenedioxy)phenyl, 261.degree.; p-tolyl, 177.degree.; 2-furly, 208.degree.; 2-thienyl, 159.degree.. A mixt. of 3.5 g. 1-tetralone and 2.5 g. 3-phenyl-1,2-dithiolium perchlorate is heated to give 2-(5-phenyl-1,2-dithiole-3-ylidene)-1-tetralone (VII), m. 139.degree. [perchlorate m. 209-10.degree. (decompn.)]. A mixt. of 100 mg. VII and 200 mg. S is heated 1 hr. at 200.degree. to give III (Ar = Ph) (VIa). Similarly prepd. are 2-[5-(p-methoxyphenyl)-1,2-dithiole-3-ylidene]-1-tetralone, m. 171.degree., and III (Ar = p-MeOC6H4). A mixt. of 1.5 g. VII, 3 g. P2S5, and 80 ml. xylene is refluxed 1 hr. to give IVa, m. 158.degree..

ACCESSION NUMBER: 1967:454060 CAPLUS
DOCUMENT NUMBER: 67:54060
TITLE: Heterocyclic sulfur compounds. XXV. Sulfuration of 2-(3-arylallylidene)-1-tetralones
AUTHOR(S): Poirier, Yves; Lozac'h, Noel
CORPORATE SOURCE: Fac. Sci. Caen, Caen, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1967), (3), 865-70
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French

IT **16209-92-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 16209-92-0 CAPLUS
CN 2-Quinolinecarboxylic acid, 7-amino-1,4-dihydro-5-hydroxy-6,8-dimethoxy-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



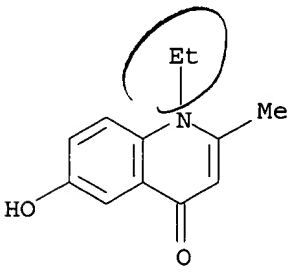
L16 ANSWER 169 OF 180 CAPLUS COPYRIGHT 2003 ACS

AB Metabolites of quinaldine-EtI (I) were investigated in the urine of rabbits by paper chromatog. As the main metabolic products the following compds. were detected: 1-ethyl-4-quinaldone (II), 1-ethyl-6-hydroxy-4-quinaldone (III), and 1-ethyl-3-hydroxy-4-quinaldone (IV). I was partly oxidized to quinaldic acid Et betaine. When II was injected, III and IV were excreted in the urine. Thus, I was oxidized to II and further oxidized to III and IV.

ACCESSION NUMBER: 1967:103740 CAPLUS
DOCUMENT NUMBER: 66:103740
TITLE: Metabolism of quinoline derivatives. Study on metabolic products of quinaldine ethiodide
AUTHOR(S): Komiyama, Zenzo
CORPORATE SOURCE: Sch. Med., Nihon Univ., Tokyo, Japan
SOURCE: Nichidai Igaku Zasshi (1964), 23(9), 541-57
CODEN: NICHAS; ISSN: 0029-0424
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

IT **15574-79-5**
RL: BIOL (Biological study)
(as quinaldine ethiodide metabolite in urine)

RN 15574-79-5 CAPLUS
CN 4(1H)-Quinolone, 1-ethyl-6-hydroxy-2-methyl- (8CI) (CA INDEX NAME)

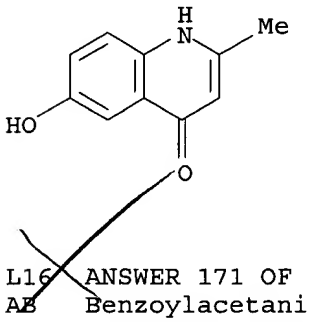


L16 ANSWER 170 OF 180 CAPLUS COPYRIGHT 2003 ACS

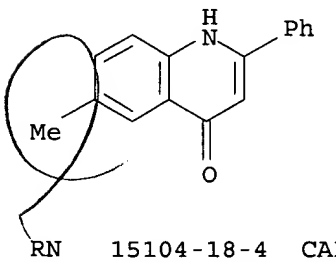
AB Metabolic products of quinaldine (I) were studied in the urine of the rabbit to which I was given s.c. and orally. 3-Hydroxyquinaldine (II), 6-hydroxyquinaldine (III), and several unknown compds. were obtained, as well as quinaldic acid (IV), as the metabolic products of I. In the case of oral administration of I, its certain fraction was excreted in the urine without any change. The unknown compds. mentioned above were not detected in the urine after injection of 4-quinaldone (V), II, III, and IV. They were not identified with compds. derived from opening of the quinoline nucleus. 6-Hydroxy-4-quinaldone and unchanged V were obtained as the metabolic products of V. II, III, and IV were excreted in the urine almost without any change, resp. These results indicate a definite difference between the metabolic pathways of I and its ethiodide (VI). Hydroxylation of VI occurred only in the 4-position of the nucleus, while that of I occurred in the 3- and 6-positions, and oxidn. occurred in the Me group.

ACCESSION NUMBER: 1967:63977 CAPLUS
DOCUMENT NUMBER: 66:63977
TITLE: Metabolism of quinoline derivatives. Metabolic products of quinaldine
AUTHOR(S): Komiya, Fukue
CORPORATE SOURCE: Sch. Med., Nihon Univ., Tokyo, Japan

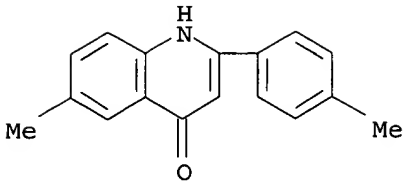
SOURCE: Nichidai Igaku Zasshi (1965), 24(7), 649-63
CODEN: NICHAS; ISSN: 0029-0424
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
IT **15502-80-4**
RL: BIOL (Biological study)
(as 4-quinaldone metabolite)
RN 15502-80-4 CAPLUS
CN 4(1H)-Quinolone, 6-hydroxy-2-methyl- (8CI) (CA INDEX NAME)



L16 ANSWER 171 OF 180 CAPLUS COPYRIGHT 2003 ACS
AB Benzoylacetanilides form 2-phenyl-4-(1H)-quinolones when acted on by an equimolar proportion of AlCl3, AlBr3, or SnCl4, BF3 affords the difluoroborane deriv. of the anilide. Complexes of the anilides with AlBr3 and SnCl4 were prepd. and heated to give the 4(1H)-quinolones. A mechanism for the anilide-quinolone transformation is suggested. 17 references.
ACCESSION NUMBER: 1967:28490 CAPLUS
DOCUMENT NUMBER: 66:28490
TITLE: Action of Lewis acids on benzoylacetanilides and related compounds
AUTHOR(S): Schiffman, B.; Staskun, B.
CORPORATE SOURCE: Univ. Witwatersrand, Johannesburg, S. Afr.
SOURCE: Tetrahedron, Supplement (1966), No. 7, 115-25
CODEN: TETSAE; ISSN: 0563-2072
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **15104-17-3P 15104-18-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 15104-17-3 CAPLUS
CN 4(1H)-Quinolinone, 6-methyl-2-phenyl- (9CI) (CA INDEX NAME)



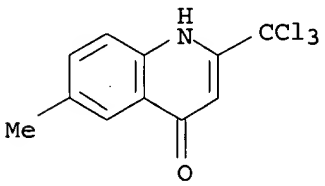
RN 15104-18-4 CAPLUS
CN 4(1H)-Quinolone, 6-methyl-2-p-tolyl- (8CI) (CA INDEX NAME)



L16 ANSWER 172 OF 180 CAPLUS COPYRIGHT 2003 ACS
GI For diagram(s), see printed CA Issue.
AB A study of the reaction of chloral and Et diazoacetate as a potential source of Et trichloroacetoacetate (I) showed that the main product of this reaction was Et 3-(trichloromethyl)glycidate. The reaction of trichloroacetyl chloride, ketene, and an alc., in liquid SO2, was found to be an excellent method to prepare trichloro-.beta.-oxo esters. The acid hydrolysis of I yielded .alpha.,.alpha.,.alpha.-trichloroacetone but this reaction could not be utilized as a general synthetic route to trichloromethyl ketones because alkylation of the ester could not be accomplished. The reactions of I with amines were studied and the products formed depended on the basicity and structure of the amine. NH3 reacted with the ester to form Et malonamate. Primary aliphatic amines yielded malonamides and secondary amines formed amine salts. Aromatic amines did not react with I under similar conditions but in the presence of polyphosphoric acid they gave 2-trichloromethyl-4-quinolones. These compds. could be hydrolyzed to kynurenic acids (II), thus providing a new synthetic route to these compds. The condensation of I with o-phenylenediamine, under neutral conditions, yielded 4-(trichloromethyl)-1H-1,5-benzodiazepin-2(3H)-one. 32 references.

ACCESSION NUMBER: 1966:499248 CAPLUS
DOCUMENT NUMBER: 65:99248
ORIGINAL REFERENCE NO.: 65:18558e-g
TITLE: Trichloroacetoacetates. I. Synthesis and reactions of ethyl and .beta.,.beta.,.beta.,-trifluoroethyl trichloroacetoacetates
AUTHOR(S): Wald, David K.; Joullie, Madeleine M.
CORPORATE SOURCE: Univ. of Pennsylvania, Philadelphia
SOURCE: J. Org. Chem. (1966), 31(10), 3369-74
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **10174-77-3**, 4(1H)-Quinolone, 6-methyl-2-(trichloromethyl)- (prepn. of)
RN 10174-77-3 CAPLUS
CN 4(1H)-Quinolone, 6-methyl-2-(trichloromethyl)- (7CI, 8CI) (CA INDEX NAME)



L16 ANSWER 173 OF 180 CAPLUS COPYRIGHT 2003 ACS

GI For diagram(s), see printed CA Issue.

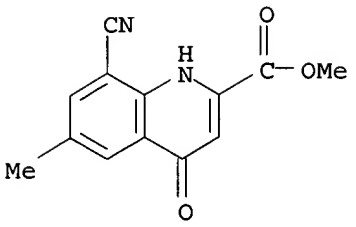
AB Certain derivs. of 3-amino- (I) and 6-aminoquinoline (II) were prepd. and tested for antiserotonin activity. To improve isolation of II from the mixt. obtained on hydrogenating 6-nitroquinoline (III), II tartrate, m. 170-1.degree., was pptd. and recrystd. I (3.6 g.) in 30 ml. 70% MeOH was treated with 5 g. NaOAc.3H2O and then 1 hr. with 6.3 g. p-MeC6H4SO2Cl, and the mixt. stirred 2 hrs. at 30-40.degree. to yield 36% IV (R = H, R1 = NHSO2C6H4Me-p), m. 172-4.degree. (MeOH). I (2.9 g.) in 40 ml. 40% AcOH diazotized at 5-8.degree. with 1.4 g. NaNO2 in 3 ml. H2O and 1 ml. HCl, the soln. stirred 30 min. and treated with 2.2 g. 2,6-diaminopyridine in 40 ml. 20% AcOH, the mixt. stirred 1 hr. at 10-12.degree. and alkalized with NH4OH yielded 3 g. V, m. 213-15.degree.. I (4.3 g.), 2.5 ml. ClCH2COCl, and 20 ml. Me2CO refluxed 45 min., the cold mixt. poured into 70 ml. H2O, the ppt. heated 3 hrs. at 60-70.degree. with 15 ml. 25% aq. Me2NH, and the soln. cooled and treated with 5 ml. satd. aq. NaOH yielded 2.5 g. IV (R = H, R1 = NHCOCH2NMe2), m. 100-1.degree. (H2O). III (17.4 g.) in 100 ml. CCl4 brominated under cooling with 16 g. Br in 25 ml. CCl4, the mixt. refluxed 1 hr., treated with boiling with 7.9 g. C5H5N in 15 ml. CCl4, and refluxed 18 hrs., and the ppt. filtered off and triturated with H2O gave 21 g. 3-bromo-6-nitroquinoline (VI), m. 170-1.degree. (AcOH). VI (10.1 g.) in 100 ml. 50% AcOH treated 30 min. at 55-60.degree. with 8 g. H-reduced Fe and the mixt. stirred 3 hrs. at 55-60.degree. and alkalized at 5-10.degree. with Na2CO3 yielded 7.5 g. IV (R = NH2, R1 = Br) (VIa), m. 154-5.degree. (MeOH). VI was also converted according to Bendz, et al. (CA 44, 10720i), into IV (R = NO2, R1 = NH2) (VII), m. 253-5.degree. and further into IV (R = NO2, R1 = NHAc) (VIII), m. 260-1.degree.. VII (5.7 g.) in 70 ml. 50% AcOH treated at 55-60.degree. with 12 g. H-reduced Fe and the mixt. heated 3 hrs. and alkalized at 5-10.degree. with Na2CO3 yielded 3.5 g. IV (R = R1 = NH2) (IX), m. 148-9.degree.. VIa (6.7 g.), 1 g. CuSO4, and 30 ml. concd. aq. NH4OH autoclaved 18 hrs. at 150-60.degree. and the mixt. alkalized with NaOH yielded 3.2 g. IX. IX was also prepd. by similarly autoclaving 3,6-dibromoquinoline. VIII (14.9 g.) reduced with Fe as described above with VI or VII yielded 4 g. IV (R = NH2, R1 = NHAc), m. 207-8.degree.. IX acetylated with Ac2O or AcCl yielded IV (R = R1 = NHAc), m. 145-7.degree., resolidifying about 150.degree., and remelting 256-8.degree.. Similarly, treatment with AcCl gave the Ac derivs. of I (HCl salt m. 280-2.degree.), II (HCl salt m. 250-3.degree.), and 8-aminoquinoline, m. 101.degree., HCl salt m. 204-5.degree.. In tests with isolated rat uterus, I was most effective (63% of the activity of lysergide). All the substituted derivs. of I and II showed poor antiserotonin activity.

ACCESSION NUMBER: 1966:456729 CAPLUS
DOCUMENT NUMBER: 65:56729
ORIGINAL REFERENCE NO.: 65:10561f-h,10562a-b
TITLE: Search for antiserotonin substances among the quinoline derivatives. I. Aminoquinolines
AUTHOR(S): Kotler-Brajtburg, Janina
CORPORATE SOURCE: Inst. Farm., Warsaw
SOURCE: Acta Polon. Pharm. (1966), 23(2), 97-103
DOCUMENT TYPE: Journal
LANGUAGE: Polish

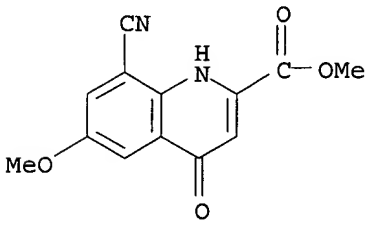
IT **7101-86-2**, Quinaldic acid, 8-cyano-1,4-dihydro-6-methyl-4-oxo-, methyl ester **7101-87-3**, Quinaldic acid, 8-cyano-1,4-dihydro-6-methoxy-4-oxo-, methyl ester **7101-88-4**, Quinaldic acid, 1,4-dihydro-6,8-dimethyl-4-oxo-, methyl ester
(prepn. of)

RN 7101-86-2 CAPLUS

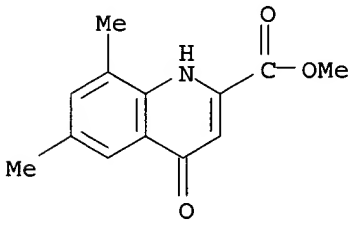
CN Quinaldic acid, 8-cyano-1,4-dihydro-6-methyl-4-oxo-, methyl ester (7CI, 8CI) (CA INDEX NAME)



RN 7101-87-3 CAPLUS
CN Quinaldic acid, 8-cyano-1,4-dihydro-6-methoxy-4-oxo-, methyl ester (7CI, 8CI) (CA INDEX NAME)

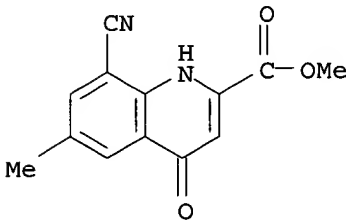


RN 7101-88-4 CAPLUS
CN Quinaldic acid, 1,4-dihydro-6,8-dimethyl-4-oxo-, methyl ester (7CI, 8CI) (CA INDEX NAME)

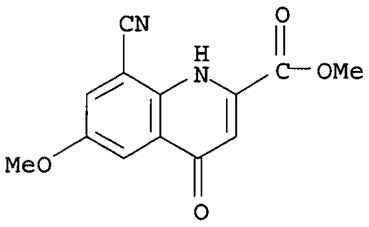


L16 ANSWER 174 OF 180 CAPLUS COPYRIGHT 2003 ACS
GI For diagram(s), see printed CA Issue.
AB Anthranilonitriles 4,2-R(NC)C6H4NH2 (I) and 2-MeOC6H4NH2 (II) and an equimolar amt. of MeO2CC.tplbond.CCO2Me refluxed in MeOH and the adducts recrystd. from MeOH gave the di-Me anilinomaleates (III, K = CN, R1 = H, Cl, Br, Me, MeO) resp. and III (R = OMe, R1 = H), m. 72-3.degree.. Pure III mixed intimately with Ph2O and refluxed over an open flame and the cooled mass dild. with excess pert. ether gave the corresponding 2-carbomethoxy-4(1H)-quinolones (IV, R = CN, R1 = H, Cl, Br, Me, MeO; R = OMe, R1 = H). Similarly was prepd. IV (R = R1 = Me, H).
ACCESSION NUMBER: 1966:456728 CAPLUS
DOCUMENT NUMBER: 65:56728
ORIGINAL REFERENCE NO.: 65:10561d-f
TITLE: Cyclization of amine-acetylene diester adducts. Modification of the Conrad-Limpach method. I
AUTHOR(S): Heindel, Ned D.; Brodof, Terry A.; Kogelschatz, Jane

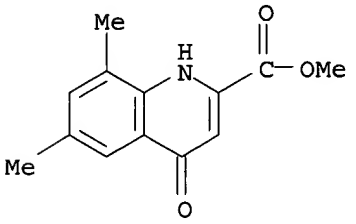
E.
CORPORATE SOURCE: Marshall Univ., Huntington, WV
SOURCE: J. Heterocyclic Chem. (1966), 3(2), 222-3
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **7101-86-2**, Quinaldic acid, 8-cyano-1,4-dihydro-6-methyl-4-oxo-, methyl ester **7101-87-3**, Quinaldic acid, 8-cyano-1,4-dihydro-6-methoxy-4-oxo-, methyl ester **7101-88-4**, Quinaldic acid, 1,4-dihydro-6,8-dimethyl-4-oxo-, methyl ester
(prepn. of)
RN 7101-86-2 CAPLUS
CN Quinaldic acid, 8-cyano-1,4-dihydro-6-methyl-4-oxo-, methyl ester (7CI, 8CI) (CA INDEX NAME)



RN 7101-87-3 CAPLUS
CN Quinaldic acid, 8-cyano-1,4-dihydro-6-methoxy-4-oxo-, methyl ester (7CI, 8CI) (CA INDEX NAME)



RN 7101-88-4 CAPLUS
CN Quinaldic acid, 1,4-dihydro-6,8-dimethyl-4-oxo-, methyl ester (7CI, 8CI) (CA INDEX NAME)

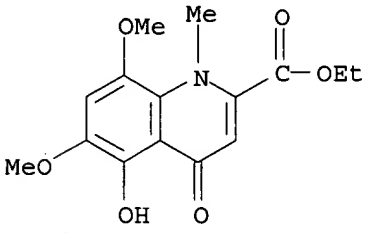


L16 ANSWER 175 OF 180 CAPLUS COPYRIGHT 2003 ACS
GI For diagram(s), see printed CA Issue.
AB The C-5 MeO group of 4-hydroxypoly-methoxyquinoline-2- and -3-carboxylic

acid esters (I) can be cleaved selectively with the retention of the ester function by BBr3. I(R = R2 = MeO, R1 = H) (II) (614 mg.) in 30 cc. dry CH2Cl2 treated with stirring at -70.degree. with 0.19 cc. BBr3, kept overnight at room temp., and evapd., and the residue refluxed 3 hrs. with 25 cc. EtOH and 2.5 cc. H2O yielded 467 mg. red III (K = R2 = MeO, R1 = H), m. 176.degree.. II (920 mg.) in 30 cc. CH2Cl2 treated dropwise with stirring at -70.degree. with 0.475 cc. BBr3, stirred 4 hrs., concd., and refluxed 4 hrs. with H2O yielded 780 mg. red 2-carbethoxy-4,5,8-trihydroxy-6-methoxyquinoline (IV), m. 173.degree. (aq. EtOH). IV (50 mg.) in 3 cc. EtOH shaken 5 min. with 150 mg. Ag2CO3 yielded 21 mg. yellow-orange 2-carbethoxy-4. hydroxy-O-methoxy-5,8-quinolinequinone, m. 212.degree. (EtOH). I((R = R1 = H, R2 = MeO) (554mg.) and 0.19 cc. BBr3 gave 379 mg. orange III (R = R1 = R2 = MeO), m. 117.degree. (CHCl3-petr. ether, b. 80-100.degree.). I (R = H, R1 = R2 = MeO) (614 mg.) with 0.19 cc. BBr3 yielded 514 mg. yellow III (R = H,R1 = R2 = MeO),m. 176.degree. (aq.EtOH). I (R = R1 = MeO, R2 = H) (307 mg.) with 0.047 cc. BBr3 in 2.5 cc. CH2Cl2 gave 241 mg. yellow III (R = R1 =MeO, R2 = H), m. 238.degree. (aq. EtOH). I (R = R1 =MeO, R2 = H) (614 mg.) in 30 cc. dry CH2Cl2 treated dropwise with stirring at room temp. with 0.095 cc. BBr3 and stirred 24 hrs., and the crude yellow-brown product refluxed 4 hrs. with 20 cc. EtOH gave 330 mg. (crude) III (R = R1 = MeO, R2 = H), m. 251.degree. (EtOH).

ACCESSION NUMBER: 1966:43685 CAPLUS
DOCUMENT NUMBER: 64:43685
ORIGINAL REFERENCE NO.: 64:8131a-d
TITLE: Selective ether cleavage of 4-hydroxymethoxyquinolinecarboxylic acid esters
AUTHOR(S): Schaefer, Wolfram; Franck, Brigitte
CORPORATE SOURCE: Max-Planck Inst. Biochem., Munich, Germany
SOURCE: Chem. Ber. (1966), 99(1), 160-4
DOCUMENT TYPE: Journal
LANGUAGE: German

IT **5237-04-7**, Quinaldic acid, 1,4-dihydro-5-hydroxy-6,8-dimethoxy-1-methyl-4-oxo-, ethyl ester
(prepn. of)
RN 5237-04-7 CAPLUS
CN Quinaldic acid, 1,4-dihydro-5-hydroxy-6,8-dimethoxy-1-methyl-4-oxo-, ethyl ester (7CI, 8CI) (CA INDEX NAME)

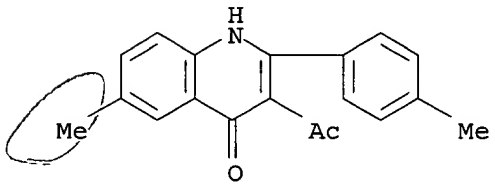


L16 ANSWER 176 OF 180 CAPLUS COPYRIGHT 2003 ACS
GI For diagram(s), see printed CA Issue.
AB Several compounds claimed to be 2-aryl-3-acetyl-4(1H)-quinolones (I) in the literature have been reformulated as the isomeric II. The conversion of 2-phenyl-3-acetyl-4-chloroquinoline to 6-phenyl-7-methyldibenzo[b,h][1,6]naphthyridine and to 2,4-diphenyl-3-methyl-2-H-pyrazolo[4,3-c]quinoline is described. .beta.-Methylamino-.alpha.-(N-arylimidoyl)crotonic esters were thermally cyclized to 2-aryl-3-N-methylacetimidoyl-4(1H)-quinolones III.

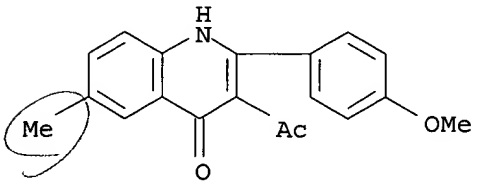
ACCESSION NUMBER: 1965:462919 CAPLUS
DOCUMENT NUMBER: 63:62919
ORIGINAL REFERENCE NO.: 63:11493a-b
TITLE: 2-Aryl-3-acetyl-4(1H)-quinolones
AUTHOR(S): Anderson, P. C.; Staskun, B.
CORPORATE SOURCE: Univ. Witwatersrand, Johannesburg, S. Afr.
SOURCE: J. Org. Chem. (1965), 30(9), 3033-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **3814-03-7**, 4(1H)-Quinolone, 3-acetyl-6-methyl-2-p-tolyl-
3814-04-8, 4(1H)-Quinolone, 3-acetyl-2-(p-methoxyphenyl)-6-methyl-
3814-05-9, 4(1H)-Quinolone, 3-acetyl-6-methoxy-2-(p-methoxyphenyl)-
3837-77-2, 4(1H)-Quinolone, 6-methoxy-2-(p-methoxyphenyl)-
(prepn. of)

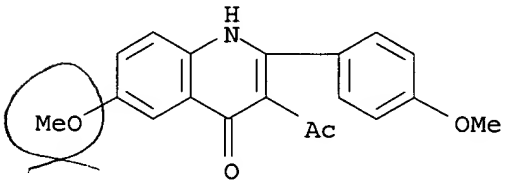
RN 3814-03-7 CAPLUS
CN 4(1H)-Quinolone, 3-acetyl-6-methyl-2-p-tolyl- (7CI, 8CI) (CA INDEX NAME)



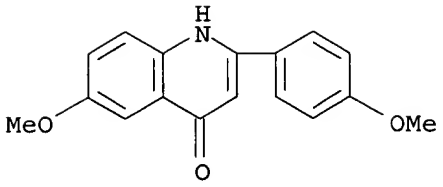
RN 3814-04-8 CAPLUS
CN 4(1H)-Quinolone, 3-acetyl-2-(p-methoxyphenyl)-6-methyl- (7CI, 8CI) (CA INDEX NAME)



RN 3814-05-9 CAPLUS
CN 4(1H)-Quinolone, 3-acetyl-6-methoxy-2-(p-methoxyphenyl)- (7CI, 8CI) (CA INDEX NAME)



RN 3837-77-2 CAPLUS
CN 4(1H)-Quinolinone, 6-methoxy-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

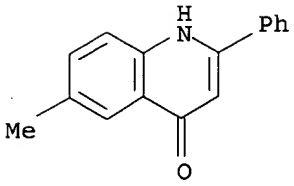


L16 ANSWER 177 OF 180 CAPLUS COPYRIGHT 2003 ACS
GI For diagram(s), see printed CA Issue.
AB 3-Chloro-3-methyl-1-butyne and NaNH2 in liquid NH3 in 5 hrs. gave 83% 3-amino-3-methyl-1-butyne (I), b. 81-2.degree., n20D 1.4216. This (10% excess) and 1,3-dimethyl-4-piperidone-MeI in H2O gave in 1 day at room temp. N-(3-methyl-1-butyn-3-yl)-3-methyl-4-piperidone (II), m. 75-7.degree.; in the presence of aq. KOH the yield was 40%; the substance also formed as follows: the quaternary salt treated with aq. KOH, followed by MeI, gave 5-dimethylamino-2-methyl-1-penten-3-one-MeI, which with I in H2O overnight gave some II. II also formed in very low yield from 5-diethylamino-4-methyl-1-pentene and I in H2O in 4 hrs. at 75.degree.. Similar treatment of I and Et2NCH2CH2COCMe:CH2 in aq. HCl gave 56% II. 2-Diethylaminoethyl 1-cyclopentenyl ketone (III) heated 2 hrs. with I in aq. HCl at 80.degree. gave some 20% N-(3-methyl-1-butyn-3-yl)perhydro-4-pyrindone (IV), m. 64.degree.. Similarly, 2-dimethylaminoethyl 1-cyclohexenyl ketone gave 54% 1-cyclohexenyl 2-(3-methyl-1-butyn-3-yl)aminoethyl ketone, isolated as the HCl salt, m. 193-5.degree.. I and Et2NCH2CH2COCMe:CHMe similarly gave N-(3-methyl-1-butyn-3-yl)-2,3-dimethyl-4-piperidone-HCl, m. 134-5.degree.; free base m. 28-9.degree.. The residue after the sepn. of the HCl salt above gave on evapn. and treatment with EtOAc some HC.tplbond.CCMe2NHCH2CH2COCMe:CHMe.HCl, m. 156-7.degree.. I and aq. CHMe:CMeCOCH:CH2 in Et2O gave in 0.5 hr. at 0.degree. and 12 hrs. at room temp., followed by heating the crude product 18 hrs. in 1:4 aq. dioxane, a 3:2 mixt. of the same products as shown above. 1,2,5-Trimethyl-4-piperidone-MeI and aq. I in 6 hrs. at 80.degree. gave some 25% N-(3-methyl-1-butyn-3-yl)-2,5-dimethyl-4-piperidone, m. 69-70.degree.. Similarly, N-methyl-4-piperidone-MeI gave N-(3-methyl-1-butyn-3-yl)-4-piperidone, m. 136.degree.. Keeping III.MeI and tert-BuNH2 in aq. soln. gave after paper chromatography of the mixt. some unsatd. material with compn. C20H31NO2, m. 150-1.degree.. The same ketone was formed when the reaction was run 3 hrs. at 80.degree..

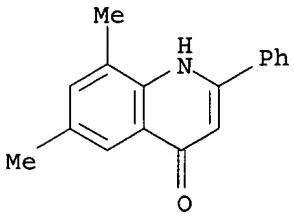
ACCESSION NUMBER: 1964:90713 CAPLUS
DOCUMENT NUMBER: 60:90713
ORIGINAL REFERENCE NO.: 60:15825b-f
TITLE: Synthesis of some substituted N-propargyl-.gamma.-piperidones
AUTHOR(S): Mistryukov, E. A.; Aronova, N. I.; Kucherov, V. F.
CORPORATE SOURCE: N. D. Zelinskii Inst. Org. Chem., Moscow
SOURCE: Izv. Akad. Nauk SSSR, Ser. Khim. (1964), (3), 512-19
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

IT **15104-17-3**, 4(1H)-Quinolone, 6-methyl-2-phenyl- **93315-55-0**, 4(1H)-Quinolone, 6,8-dimethyl-2-phenyl-
(prepn. of)

RN 15104-17-3 CAPLUS
CN 4(1H)-Quinolinone, 6-methyl-2-phenyl- (9CI) (CA INDEX NAME)



RN 93315-55-0 CAPLUS
CN 4(1H)-Quinolinone, 6,8-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)

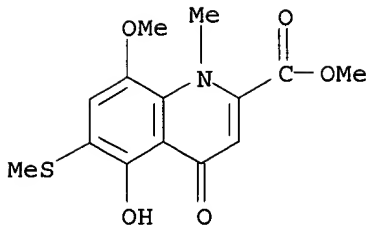


L16 ANSWER 178 OF 180 CAPLUS COPYRIGHT 2003 ACS
GI For diagram(s), see printed CA Issue.
AB 4,5,8-Trihydroxy-6-mercaptoquinoline-2-carboxylic acid (Ia) (R = SH, R1 = H) (I) was prepd. by cleavage of Ia (R = EtOCS2, R1 = Et) (II) with AlBr3. Cleavage of I with HBr resulted in reductive cleavage of the S function. Methylation of I with CH2N2 yielded 2-carbomethoxy-4,5,8-trimethoxy-6-methylthioquinoline (III) and IV. Contrary to expectations, I is not identical with a degradation product from the ommochrome, ommine A (CA 53, 10580i). 2,5-(HO)2C6H3SH (24 g.) in 200 cc. 9N KOH with 160 g. Me2SO4 under N yielded 18 g. 2,5-(MeO)2C6H3SMe (V), b0.07 96-79, m. 35.degree.. V (20 g.)in 200 cc. AcOH and 20 cc. 65% HNO3 in 20 cc. AcOH kept 1 hr. at 5.degree. yielded 20 g. 2,5,4-(MeO)2(MeS)C6H2NO2 (VI), m. 174.degree. (EtOH). 2,5,4-(MeO)2(O2N)C6H2NH2 (VII) (9.5 g.), 70 cc. concd. HCl, and 100 cc. H2O diazotized at 0-3.degree. with 3.2 g. NaNO2 in 100 cc. H2O, adjusted with 33 g. Na2CO3 at -2.degree. to pH 3.5, added at 70.degree. to a soln. of 25 g. EtOCS2K under 700 cc. MePh, and the crude product refluxed 40 min. under N with 200 cc. EtOH and 10 g. KOH and then treated with 30 cc. Me2SO4 and 10% aq. KOH yielded 5 g. VI. VI (10 g.) in dry tetrahydrofuran hydrogenated with Raney Ni under ambient conditions yielded 2,5,4-(MeO)2(MeS)C6H2NH2 (VIII), which is sensitive to air. VIII (9.1 g.) and 9.5 g. EtO2CCOCH2CO2Et heated 2 hrs. under N on the steam bath gave 7.4 g. yellow IX, m. 87-8.degree.; orange crystals m. 90-2.degree. (EtOH). IX (2 g.) in 6 cc. Dowtherm added dropwise with stirring at about 250.degree. to 20 cc. Dowtherm, the mixt. kept 10 min. at 250.degree., cooled to 90.degree., and dild. dropwise with 20 cc. ligroine (b. 50-80.degree.) gave 89% 4-OH analog (X) of III, m. 149.degree. (AcOEt). X (800 mg.) and 50 cc. 48% HBr refluxed 3 hrs., yielded 300 mg. red Ia.HBr (R = MeS, R1 = H) (XI.HBr), decomp. 295.degree. (aq. EtOH). X (500 mg.) and 15 cc. azeotropic HI refluxed 4 hrs. under N yielded 280 mg. 4,5,8-trihydroxyquinoline-2-carboxylic acid (XII), decomp. 295.degree.. 4-Hydroxy-5,8-dimethoxy-2-carbethoxyquinoline (XIII) (18 g.) in 180 cc. AcOH added dropwise at 15.degree. to 24 cc. AcOH and 24 cc. 86% HNO3, and kept 1 hr. at 15.degree. yielded 19.1 g. 6-NO2 deriv. (XIV) of XIII, m. 192-3.degree. (EtOH). VII (10 g.) and 10.5 g. EtO2CCOCH2CO2Et heated 2 hrs. at 130.degree. under N, treated with an addnl. 10 g.

EtO2CCOCH2CO2Et, and heated again 2 hrs. at 150-60.degree. yielded 2.8 g. XV, decomp. 226.degree. (AcOEt). XV (220 mg.) in 12 cc. hot Dowtherm added dropwise to 50 cc. refluxing Dowtherm and refluxed 0.5 hr. yielded 30 mg. XIV, m. 190.degree., and some VII. XIV (8.5 g.) in EtOH hydrogenated under ambient conditions over Raney Ni yielded 4.8 g. yellow-red 6-NH2 deriv. (XVI), m. 171.degree. (AcOEt). XVI (6.3 g.) in 1 l. H2O and 175 cc. concd. HCl diazotized at -2 to 0.degree. with 22 g. NaNO2, adjusted with about 100 g. Na2CO3 to pH 4, added to 100 g. EtOCS2K in 600 cc. H2O and 1.5 l. MePh, adjusted with about 20 cc. AcOH to pH 8, and stirred 1 hr. at 75-80.degree. yielded about 30 g. mixt. of II and Ia (R = SCO2Et, R1 = Et) (XVII) and 4 g. XIII; the II-XVII mixt. recrystd. from 0.7 l. (iso-Pr)2O and a 370mg. portion chromatographed on 100 g. silica gel yielded 170 mg. II, m. 132-3.5.degree. (1:5 CCl4-cyclohexane), 100 mg. II-XVII mixt., and 50 mg. XVII, m. 169-71.degree.. II (200 mg.) and 600 mg. KOH in 20 cc. MeOH and 20 cc. H2O refluxed 0.5 hr. under N, the mixt. cooled, treated with 4 cc. Me2SO4, the yellow ppt. dissolved in 15 cc. satd. alc. HCl, kept overnight, and refluxed 2 hrs. gave 50 mg. X, m. 148.degree.. II-XVII mixt. (1.2 g.) refluxed 2 hrs. with 90 cc. 48% HBr gave 300 mg. XII. 2,5-(MeO)2C6H3-NH2 (15.3 g.) in 150 cc. 4N HCl diazotized at 0-2.degree. with 7 g. NaNO2, adjusted with Na2CO3 to pH 4, and added at 70-80.degree. to 20 g. EtOCS2K in H2O and 200 cc. MePh gave 3 g. [2,5-(MeO)2-C6H3S]2CO, m. 116-17.degree. (EtOH), Rf 0.1 (1:1 C6H6-cyclohexane, thin-layer), and a mixt. which chromatographed on silica gel yielded about 750 mg. dixanthogen, Rf 0.9, and 4.5 g. oily 2,5(MeO)2C6H3S2COEt (XIX), Rf 0.5. XIX (1 g.) in 25 cc. dry C6H6 refluxed 3 hrs. under N with 16.6 cc. AlBr3-C6H6 (250 mg./cc.) gave 420 mg. 2,5-(HO)2C6H3SH. II-XVII mixt. (600 mg.) in 20 cc. dry C6H6 treated dropwise at room temp. with 10 cc. 25% AlBr3-C6H6, and the pptd. complex washed with C6H6 and decompd. with 50 cc. 0.1N HCl yielded 370 mg. red-orange I.H2O, decomp. from 290.degree. with darkening (aq. MeOH), Rf 0.36 (4:1:1.5 BuOH-AcOH-H2O). I (5 mg.) in 20 cc. EtOH refluxed 2 hrs. with Raney Ni gave about 2 mg. XII. I (8 mg.) in 10 cc. 48% HBr refluxed 45 min. under CO2 yielded 4 mg. XII. I (95 mg.) in 5 cc. MeOH treated 1 day at 0.degree. and 2 days at room temp. with CH2N2-Et2O yielded 40 mg. IV [m. 162-3.degree. (MeOH), Rf 0.8], 15 mg. viscous, yellow sirup, and 50 mg. III. X (1.1 g.) in 150 cc. abs. MeOH satd. at 10.degree. with dry HCl, kept 2 days at room temp., and refluxed 3 hrs. yielded 920 mg. (crude) 6-MeS deriv. (XX) of XIII, m. 179-81.degree.. XX (300 mg.) in 50 cc. MeOH treated 1 day at room temp. with excess CH2N2-Et2O yielded 200 mg. III, m. 174-5.degree. (1:2 C6H6-cyclohexane).

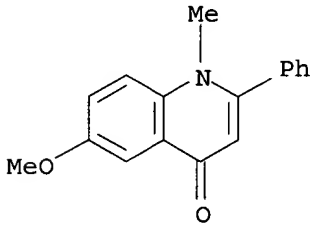
ACCESSION NUMBER: 1964:38689 CAPLUS
DOCUMENT NUMBER: 60:38689
ORIGINAL REFERENCE NO.: 60:6818g-h,6819a-h
TITLE: Preparation and conversions of 4,5,8-trihydroxy-6-mercaptoquinoline-2-carboxylic acid
AUTHOR(S): Butenandt, Adolf; Biekert, Ernst; Haerle, Eckhart
CORPORATE SOURCE: Max-Planck-Inst. Biochem., Munich, Germany
SOURCE: Ber. (1964), 97(1), 285-94
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

IT **93004-98-9**, Quinaldic acid, 1,4-dihydro-5-hydroxy-8-methoxy-1-methyl-6-(methylthio)-4-oxo-, methyl ester
(prepn. of)
RN 93004-98-9 CAPLUS
CN Quinaldic acid, 1,4-dihydro-5-hydroxy-8-methoxy-1-methyl-6-(methylthio)-4-oxo-, methyl ester (7CI) (CA INDEX NAME)



L16 ANSWER 179 OF 180 CAPLUS COPYRIGHT 2003 ACS
AB cf. preceding abstr. 6-Methoxy-2-phenyl-4-quinolinol (I), m. 309-12.degree., was formed in 50% yield by treating p-anisidine and ethyl benzoylacetate in azeotropic chloroform, followed by cyclizing in refluxing Dowtherm at 255-60.degree.. Subsequent treatment of I with Me2SO4 and 30% NaOH gave 6-methoxy-1-methyl-2-phenyl-4-quinolone, m. 186-7.degree., identical with eduline from C. edulis.

ACCESSION NUMBER: 1961:54399 CAPLUS
DOCUMENT NUMBER: 55:54399
ORIGINAL REFERENCE NO.: 55:10488b-c
TITLE: Structure and synthesis of eduline. Alkaloids of Casimiroa edulis
AUTHOR(S): Beyerman, H. C.; Rooda, R. W.
CORPORATE SOURCE: Tech. Hogeschool, Delft, Neth.
SOURCE: Koninkl. Ned. Akad. Wetenschap., Proc., Ser. B (1960), 63, 432-3
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **6878-08-6**, Eduline
(structure of)
RN 6878-08-6 CAPLUS
CN 4(1H)-Quinolinone, 6-methoxy-1-methyl-2-phenyl- (9CI) (CA INDEX NAME)



L16 ANSWER 180 OF 180 CAPLUS COPYRIGHT 2003 ACS
AB cf. Power and Callan, C.A. 6, 667. The dried, ground kernels were extd. twice with 400 l. hot EtOH. The combined exts. were evapd. and dild. with 50 1.4% aq. HCl. The mixt. was extd. (5 .times. 101. each) with C6H14 (A), C6H6 (B), CH2Cl2 (C), and AmOH (D). The aq. layer was basified with aq. NH3 and extd. similarly to give the basic exts. (E, F, G, and H), resp. A was chromatographed on 40 parts of Al2O3. Elution with 7:3 C6H6-Et2O gave .beta.-sitosterol, m. 138-9.degree., [.alpha.]D -38.degree.; acetate, m. 127-8.degree., [.alpha.]D -38.degree.; benzoate, m. 145-7.degree., [.alpha.]D -12.degree.. Further elution with 1:1 C6H6-Et6O gave palmitamide, m. 103-4.degree.. Chromatography of B and elution with 4:1 C6H6-Et6O gave zapotin, C19H18O6 (I), m. 150-1 (picrate, m. 181-2.degree.; perchlorate, m. 204-6.degree.; oxime, m. 240-3.degree.);

3:1 C6H6-Et2O gave casimiroin, C12H11NO4 (II), m. 202-3.degree. (picrate, m. 193-4.degree.; aurichloride, m. 196-8.degree.); 4:1 Et2O-EtOAc gave N-benzoyltyramine (III), m. 161-2.degree. (acetate, m. 121-2.degree.; benzoate, m. 172-3.degree.). I (4 g.) was refluxed 1 hr. with 60 ml. Ac2O and 85 ml. aq. HI to yield 3.1 g. of demethylzapotin, C15H10O6 (IV), m. 321-5.degree., green with alc. FeCl3. KOH-fusion of IV yielded salicylic acid, m. 156-8.degree., and resorcinol (dibenzoate, m. 116.5.degree.). Refluxing II 20 min. in 20% aq. HCl gave casimiroinol, C11H9NO4 (V), m. 321-3.degree.. V with CH2N2 gave II. KOH-fusion of III gave BzOH. III with CH2N2 gave the Me ether, m. 123-4.degree. which was oxidized with alk. KMnO4 to give p-MeOC6H4CO2H. C yielded 9-hydroxy-4-methoxyfurano[3,2-g]benzopyran-7-one (VI), m. 223-4.degree.; acetate, m. 181-2.degree. benzoate, m. 203-5.degree.. VI with CH2N2 gave isopimpinellin, C13H10O5, m. and mixed m.p. 150-1.degree.. VI with CrO3-AcOH gave bergaptenquinone, m. 251-3.degree. (decompn.). VI in alk. KMnO4 gave 2,3-furandicarboxylic acid, m. 220-1.degree.. Chromatography of the mother liquor from C and elution with C6H6 gave zapotinin, C18H16O6 (VII), m. 224-5.degree. green with alc. FeCl3 (acetate, m. 214-16.degree.); C6H6-CH2Cl2 gave zapoterin, C19H24O6 (VIII), m. 257-9.degree. [.alpha.]D -51.degree.; CH2Cl2 gave casmirolid, m. 229-31, [.alpha.]D -49.degree.. KOH-fusion of I at 270.degree. for 20 min. gave VII. IV with CH2N2 also gave VII. VIII kept 1 hr. with Ac2O and C5H5N at 90.degree. gave isozapoterin, m. 284-5.degree.. D sepd. .beta.-sitosterol .beta.-D-glucoside, m. 290-5.degree. (decompn.); tetraacetate, m. 164-6.degree.. Chromatography of F and elution with 9:1 C6H6-Et2O gave eduline, C17H15-NO2, m. 187-8.degree.; picrate, m. 225-7.degree. perchlorate, m. 250-2.degree.. Chromatography of G and elution with C6H6 gave zapotidine, C7H9N3S, m. 96-8.degree.; picrate, m. 195-6.degree.. H crystd. casimiroedine, C17H24N2O5, m. 224-5.degree., [.alpha.]D -33.degree..

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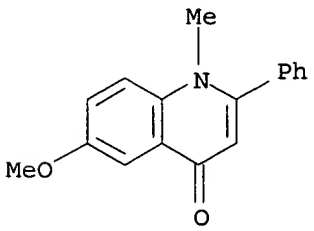
CN 4(1H)-Quinolinone, 6-methoxy-1-methyl-2-phenyl- (9CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	97.34	292.82

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-13.67	-13.67

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